

ChE-601

Hands-on with Research Data Management in Chemistry

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Cursus	Sem.	Type
Chemistry and Chemical Engineering		Opt.

Language of teaching	English
Credits	1
Session	
Exam	Project report
Workload	30h
Hours	24
Lecture	12
Exercises	3
Practical work	9
Number of positions	15

Frequency

Every year

Remark

Next time Winter 24 (block)

Summary

PhD students in Chemistry will learn hands-on Research Data Management (RDM) skills transferable to their research practices. They will contextualize their research into RDM best practices (day 1), discover appropriate tools (day 2) and work on a project (day 3) for the course accreditation

Content**DAY 1: RDM GOOD PRACTICES & EPFL SOLUTIONS**

Main scope: PhD students will contextualize their current lab RDM practices in light of FAIR principles

- Contextualize the FAIR data principles in the chemical research field
- Discover the SNSF DMP as a guideline
- Differentiate between raw data, processed data and code
- Compare ELNs and other collaborative solutions
- Collaborative tools:
 - Collaborative writing tools (Authorea, Overleaf, HackMD, ...)
 - Electronic Lab Notebooks (EPFL ELN, SLIMs, OpenBis, ...)
 - Cloud storage solutions (Switch, EPFL GDrive, OwnCloud, ...)
- Data organization, file naming and documentation
- Discover metadata for research data

DAY 2: TOOLS HANDS-ON

Main scope: PhD students will discover software and platforms to improve their current RDM practices

- Data formats, exporting & conversion
- Differentiate between storage, back-up and preservation solutions
- Data reuse:
 - Discover the re3data.org
 - Data access & re-use from data repositories
- Versioning:
 - Git
- Data manipulation
 - Dataviz for publication
 - Open tools for data analysis
 - Data formats converters

Practical session: PhD students will model and present their current practices and workflows involving research data

DAY 3: PROJECT

Main scope: PhD students will discover further tools and concepts to plan their RDM activities and improve their research workflows

- Dealing with sensitive data, proprietary data and licensing
- Data publishing via data repositories, data archiving
- Computational chemistry workflows and tools

Practical session: PhD students will refine their workflow models and present them for peer-assessment and evaluation

- Pitch the RDM aspects of the research project
- Describe data generation & reuse
- Select relevant and applicable solutions for their project, such as:
 - storage & collaborative tools
 - documentation & metadata standards
 - repositories for data publication and archiving

Learning Outcomes

By the end of the course, the student must be able to:

- Define Data Life-Cycle of his/her research
- Identify Specific softwares
- Apply RDM good practices

Resources**Moodle Link**

- <https://go.epfl.ch/ChE-601>